JOURNAL OF MATHEMATICAL PHYSICS VOLUME 9, NUMBER 7 JULY 1968

Mean Entropy of States in Quantum-Statistical Mechanics

OSCAR E. LANFORD III
University of California, Berkeley, California

AND

DEREK W. ROBINSON
CERN, Geneva

(Received 6 September 1967)

The equilibrium states for an infinite system of quantum mechanics may be represented by states over suitably chosen C^* algebras. We consider the problem of associating an entropy with these states and finding its properties, such as positivity, subadditivity, etc. For the states of a quantum-spin system, a mean entropy is defined and it is shown that this entropy is affine and upper semicontinuous.

1. INTRODUCTION

In the algebraic theory of statistical mechanics the class of possible equilibrium states is defined as the subclass K of states ρ, over the C^* algebra $\mathcal{A}$ of local observables, which satisfy certain subsidiary conditions of a physical origin. Firstly, it is assumed that the theory is invariant under a symmetry group G (the translation group R^ν, for example), and the states $\rho \in K$ considered are taken to be G invariant. Secondly, as one wishes to describe only systems with a finite number of particles in each finite subsystem, extra conditions must be introduced. The consequence of these latter "finite mean density" conditions can be described as follows: If $\Lambda \subset R^\nu$ is an open set of compact closure and $\mathcal{A}(\Lambda) \subset \mathcal{A}$ is the corresponding subalgebra of strictly local observables, then a state $\rho \in K$ must be such that its restriction to each $\mathcal{A}(\Lambda)$ is described by a density matrix ρ_Λ acting on a Hilbert space $\mathcal{H}_\Lambda$. As a direct result of this last property we may introduce, for each $\rho \in K$, a family of entropies $S(\rho_\Lambda)$ by the definition

$$S(\rho_\Lambda) = -\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda).$$

Consequently, we may study properties of $S(\rho_\Lambda)$, attempt to introduce for each $\rho \in K$ an entropy per unit volume $S(\rho)$, and, subsequently, analyse the linearity and continuity properties, etc., of $S(\rho)$.

The program outlined above was recently completed by Ruelle, in collaboration with one of the present authors (D. W. R.), in the framework of classical statistical mechanics.[1] The purpose of the present paper is to attempt the same program for quantum-statistical mechanics. In this latter setting many difficulties arise due to noncommutativity, and our results are complete only for quantum-spin systems. In the general case many interesting problems remain open.

[1] D. W. Robinson and D. Ruelle, Commun. Math. Phys. 5, 288 (1967).

2. GENERAL FORMULATION

We want to investigate both continuous infinite quantum-statistical systems and lattice systems. Thus, we consider a C^* algebra $\mathcal{A}$ and a collection $\{\mathcal{A}(\Lambda)\}$ of C^* subalgebras of $\mathcal{A}$, where Λ runs over:

(i) the bounded open sets in R^ν for continuous systems;

(ii) the finite subsets of Z^ν for lattice systems.

We suppose that these subalgebras satisfy the following axioms:

(1) $\mathcal{A}(\Lambda_1) \subset \mathcal{A}(\Lambda_2)$ if $\Lambda_1 \subset \Lambda_2$.

(2) For each Λ, $\mathcal{A}(\Lambda)$ is isomorphic to $\mathcal{L}(\mathcal{H}_\Lambda)$ for some Hilbert space $\mathcal{H}_\Lambda$. We will usually identify $\mathcal{A}(\Lambda)$ with $\mathcal{L}(\mathcal{H}_\Lambda)$, although this is not strictly compatible with axiom (1).

(3) $\mathcal{A}$ is the norm closure of $\cup_\Lambda \mathcal{A}(\Lambda)$.

(4) $\mathcal{A}(\Lambda_1 \cup \Lambda_2)$ is generated by $\mathcal{A}(\Lambda_1) \cup \mathcal{A}(\Lambda_2)$ in the weak operator topology on $\mathcal{L}(\mathcal{H}_{\Lambda_1 \cup \Lambda_2})$.

(5) Let G denote the group of translations, i.e., $G = Z^\nu$ for lattice systems and $G = R^\nu$ for continuous systems. Then G acts on $\mathcal{A}$ by automorphisms τ_x in such a way that $\tau_x(\mathcal{A}(\Lambda)) = \mathcal{A}(\Lambda + x)$ for all regions Λ and translations x.

Finally, we need a condition expressing the independence of observables belonging to disjoint regions. This condition may take one of two forms, depending on whether we are considering bosons or fermions:

(6) Either

(a) If Λ_1 and Λ_2 are any two disjoint regions, then $\mathcal{A}(\Lambda_1)$ commutes with $\mathcal{A}(\Lambda_2)$; or

(b) Each $\mathcal{A}(\Lambda)$ is generated by a set of creation and annihilation operators satisfying the canonical anticommutation relations, and, if Λ_1 and Λ_2 are disjoint regions, the creation and annihilation operators for Λ_1 anticommute with those for Λ_2.

These axioms describe several kinds of physical systems:

(1) Ordinary continuous quantum systems, either bosons or fermions.

(2) Quantum lattice systems, again either bosons or fermions, with finitely many creation and annihilation operators associated with each lattice site. For fermion lattice systems, $\mathcal{H}_\Lambda$ is finite-dimensional for each finite set Λ, but for boson systems this is, of course, not true.

(3) Quantum-spin systems. In this case, $\mathcal{H}_\Lambda$ is finite-dimensional for each bounded region Λ, but the different unit rays in $\mathcal{H}_{\{x\}}$, where x is a lattice point, are interpreted as describing different polarization states of a particle localized at x rather than varying occupation numbers for that point. We will assume that such systems satisfy axiom (6a).

The statistical-mechanical states of $\mathcal{A}$ are those which, when restricted to an $\mathcal{A}(\Lambda)$, are given by a density matrix. In other words, such a state ρ defines, for each region Λ, a positive operator ρ_Λ on $\mathcal{H}_\Lambda$, with $\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda) = 1$, such that

$$\rho(A) = \mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda A),$$

if $A \in \mathcal{A}(\Lambda) = \mathfrak{L}(\mathcal{H}_\Lambda)$. This statement imposes no restriction on ρ if $\mathcal{H}_\Lambda$ is finite-dimensional; otherwise, it corresponds to the requirement that there be only finitely many particles in the region Λ.

Every statistical-mechanical state ρ defines a family $\{\rho_\Lambda\}$ of density matrices. Conversely, the assignment of a density matrix to each bounded region defines a statistical-mechanical state on $\mathcal{A}$, provided that the assignment satisfies the obvious compatibility condition that, if $\Lambda_1 \subset \Lambda_2$ and if $A \in \mathcal{A}(\Lambda_1)$, then

$$\mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}(\rho_{\Lambda_1} A) = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_2} A).$$

We can reformulate the compatibility condition as follows: If $\Lambda_1 \subset \Lambda_2$, then $\mathcal{A}(\Lambda_1)$ is a type I factor contained in $\mathcal{A}(\Lambda_2) = \mathfrak{L}(\mathcal{H}_{\Lambda_2})$. Hence, we may factorize

$$\mathcal{H}_{\Lambda_2} = \mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$$

in such a way that an operator A in $\mathcal{A}(\Lambda_1) = \mathfrak{L}(\mathcal{H}_{\Lambda_1})$ is identified with the operator $A \otimes 1$ on $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$. [The space $\mathcal{H}'$ may be identified with $\mathcal{H}_{\Lambda_2 - \Lambda_1}$, but operators in $\mathcal{A}(\Lambda_2 - \Lambda_1)$ do not factorize as nicely as those in $\mathcal{A}(\Lambda_1)$ unless algebras for disjoint regions commute. See below.] The compatibility condition may now be formulated as

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}'}(\rho_{\Lambda_2}),$$

where $\mathrm{Tr}_{\mathcal{H}'}$ means the partial trace with respect to $\mathcal{H}'$, i.e., if $\{\varphi_i\}$ is an orthonormal basis for $\mathcal{H}_{\Lambda_1}$ and $\{\psi_i\}$ is an orthonormal basis for $\mathcal{H}'$, then

$$(\rho_{\Lambda_1}\varphi_i, \varphi_k) = \sum_{j=1}^{\infty} [\rho_{\Lambda_2}(\varphi_i \otimes \psi_j), \varphi_k \otimes \psi_j].$$

The condition that a state be translation-invariant may easily be formulated in terms of the corresponding system of density matrices. For any region Λ and any translation x, τ_x is an isomorphism of $\mathcal{A}(\Lambda)$ onto $\mathcal{A}(\Lambda + x)$. Since $\mathcal{A}(\Lambda)$ is identified with $\mathfrak{L}(\mathcal{H}_\Lambda)$ and $\mathcal{A}(\Lambda + x)$ with $\mathfrak{L}(\mathcal{H}_{\Lambda+x})$, there is a unitary operator $U_{\Lambda,x}$ from $\mathcal{H}_\Lambda$ to $\mathcal{H}_{\Lambda+x}$ which induces this isomorphism, and $U_{\Lambda,x}$ is determined up to a multiplicative constant. Then the state defined by the system $\{\rho_\Lambda\}$ of density matrices is translation-invariant if and only if

$$\rho_{\Lambda+x} = U_{\Lambda,x}\rho_\Lambda U_{\Lambda,x}^{-1},$$

for all regions Λ and translations x.

We now want to make a more careful analysis of the relation of $\rho_{\Lambda_1 \cup \Lambda_2}$ to ρ_{Λ_1} and ρ_{Λ_2} when Λ_1 and Λ_2 are disjoint regions. We have already remarked that the inclusion of $\mathcal{A}(\Lambda_1)$ in $\mathcal{A}(\Lambda_1 \cup \Lambda_2)$ gives a factorization of $\mathcal{H}_{\Lambda_1 \cup \Lambda_2}$ as $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$, where operators in $\mathcal{A}(\Lambda_1)$ go over into operators of the form $A \otimes 1$. If we are considering a boson system or a spin system, then the commutant of $\mathcal{A}(\Lambda_1)$ in $\mathcal{A}(\Lambda_1 \cup \Lambda_2)$ is precisely $\mathcal{A}(\Lambda_2)$. In this case, there is an essentially unique way to identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$, and operators in $\mathcal{A}(\Lambda_2)$ take the form $1 \otimes A$ on $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$. Hence we have

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_1 \cup \Lambda_2}), \quad \rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}(\rho_{\Lambda_1 \cup \Lambda_2}).$$

For fermion systems, although $\mathcal{H}'$ has the same dimension as $\mathcal{H}_{\Lambda_2}$, there is no unique sensible way to identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$. Nevertheless, by using the special structure of fermion systems, we can construct a useful identification of $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$. This we do as follows: Let N_1 and N_2 denote the number operators for the regions Λ_1 and Λ_2, respectively. Then a simple calculation with the anticommutation relations shows that the commutant of $\mathcal{A}(\Lambda_1)$ in $\mathcal{A}(\Lambda_1 \cup \Lambda_2)$ is precisely $(-1)^{N_1 N_2}\mathcal{A}(\Lambda_2)(-1)^{N_1 N_2}$. Therefore, we can identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$ in such a way that if A is in $\mathcal{A}(\Lambda_2) = \mathfrak{L}(\mathcal{H}_{\Lambda_2})$, then A goes over into

$$(-1)^{N_1 N_2}(1 \otimes A)(-1)^{N_1 N_2},$$

in $\mathfrak{L}(\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2})$. With this identification we have

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_1 \cup \Lambda_2}),$$
$$\rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}[(-1)^{N_1 N_2}\rho_{\Lambda_1 \cup \Lambda_2}(-1)^{N_1 N_2}].$$

The second of these equations can be simplified if we assume that ρ is an even state of $\mathcal{A}$. By definition, an element A of some $\mathcal{A}(\Lambda)$ is *odd* if

$$(-1)^{N(\Lambda)}A(-1)^{N(\Lambda)} = -A,$$

where $N(\Lambda)$ is the number operator for the region Λ. A state ρ of $\mathcal{A}$ is *even* if ρ vanishes on every odd element of every $\mathcal{A}(\Lambda)$. If ρ is now an even state and A is an element of $\mathcal{A}(\Lambda_2)$, then

$$\rho(A) = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}}[\rho_{\Lambda_1 \cup \Lambda_2}(-1)^{N_1 N_2}(1 \otimes A)(-1)^{N_1 N_2}]$$
$$= \mathrm{Tr}_{\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}}[\rho_{\Lambda_1 \cup \Lambda_2}(1 \otimes A)].$$

To prove this equation, note that we can write A as the sum of an even part and an odd part, that the odd part contributes nothing to $\rho(A)$, and that the even part commutes with $(-1)^{N_1 N_2}$. Collecting these results we have:

Proposition 1: Let ρ be a statistical-mechanical state of the C^* algebra $\mathcal{A}$, and let $\{\rho_\Lambda\}$ be the corresponding system of density matrices. If $\mathcal{A}$ is the algebra for a fermion system, we further assume that ρ is even. Then, if Λ_1 and Λ_2 are disjoint regions, we may identify $\mathcal{H}_{\Lambda_1 \cup \Lambda_2}$ with $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$ in such a way that

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_1 \cup \Lambda_2}) \quad \rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}(\rho_{\Lambda_1 \cup \Lambda_2}).$$

Note that if we are dealing with a fermion system, then translation invariance implies that the state ρ is even. To show this[2] let A be an odd element of some $\mathcal{A}(\Lambda)$ and let x be a translation large enough so that $\Lambda + nx$ does not intersect Λ for $n = 1, 2, 3, \cdots$ Let

$$A_N = \frac{1}{N} \sum_{n=0}^{N-1} \tau_{nx} A.$$

Now

$$\begin{aligned} \|A_N\|^2 = \|A_N^* A_N\| &\le \|\{A_N^*, A_N\}\| \\ &\le \frac{1}{N^2} \sum_{n,m=0}^{N-1} \|\{(\tau_{nx}A)^*, \tau_{mx}A\}\| \\ &\le \frac{2}{N} \|A\|^2, \end{aligned}$$

where the last inequality is a consequence of

$$\{(\tau_{nx}A)^*, \tau_{mx}A\} = 0, \quad \text{for} \quad n \ne m.$$

However, by translation invariance,

$$\rho(A) = \rho(A_N) = \lim_{N\to\infty} \rho(A_N).$$

But as $\lim_{N\to\infty} \|A_N\| = 0$, then $\lim_{N\to\infty} \rho(A_N) = 0$ and thus $\rho(A) = 0$.

Given a statistical-mechanical state ρ and a region Λ, we can define the entropy of the region Λ as follows:

$$\begin{aligned} S(\rho_\Lambda) &= +\infty, \text{ if } \rho_\Lambda \log \rho_\Lambda \text{ is not of trace class on } \mathcal{H}_\Lambda \\ &= -\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda), \text{ otherwise.} \end{aligned}$$

In defining the operator $\rho_\Lambda \log \rho_\Lambda$ we use the usual convention $x \log x = 0$, for $x = 0$.

3. BASIC INEQUALITIES FOR THE ENTROPY

Lemma 1[3]*:* If A and B are positive, self-adjoint, trace-class operators on a Hilbert space $\mathcal{H}$, then

$$\mathrm{Tr}_{\mathcal{H}}[A \log A - A \log B - A + B] \ge 0.$$

[2] This proof was independently discovered by R. T. Powers.

[3] This lemma, together with its proof, was communicated to one of us (D. W. R.) by Professor R. Jost, who attributed it to O. Klein. If $\mathrm{Tr}(A) = \mathrm{Tr}(B) = 1$, this lemma is a particular case of Theorem 1 of H. Umegaki, Kodai Math. Sem. Rep. **14**, 59 (1962).

Proof: Let $\psi_i(\varphi_i)$ be a complete orthonormal set of eigenfunctions of $A(B)$ and let $a_i(b_i)$ be the corresponding eigenvalues. Let $U = (U_{ij})$ be a unitary mapping defined by

$$\psi_i = \sum_j U_{ij} \varphi_j.$$

Now

$$\begin{aligned} (\psi_i | A \log A - A \log B | \psi_i) &= a_i \Big\{ \log a_i - \sum_j |U_{ij}|^2 \log b_j \Big\} \\ &\ge a_i \Big\{ \log a_i - \log \sum_j |U_{ij}|^2 b_j \Big\} \\ &\ge a_i - \sum_j |U_{ij}|^2 b_j \\ &= (\psi_i | A - B | \psi_i), \end{aligned}$$

where, to obtain the first inequality, we have used the concavity of the logarithm and, to obtain the second inequality, we have used

$$\log x \ge 1 - 1/x \quad (x > 0).$$

The result follows by summation.

Lemma 2: If A and B be positive, self-adjoint operators on a Hilbert space $\mathcal{H}$, then, for $1 \ge \alpha \ge 0$,

$$[\alpha A + (1-\alpha)B] \log [\alpha A + (1-\alpha)B] \le \alpha A \log A + (1-\alpha) B \log B,$$

and furthermore

$$A \ge B \ge 0 \quad \text{implies} \quad \log A \ge \log B.$$

The statements of the lemma are special consequences of the theory of convex and monotone operator functions initially developed by Löwner.[4] For further results, the reader may consult Ref. 5. The details of the application of the general theory to the case at hand are worked out in Refs. 6 and 7. Moreover, we do not need the full force of the first inequality of the lemma, but only the inequality obtained by taking its trace; this latter inequality can be proved without use of the general theory of convex operator functions.[7,8]

We remark that Lemma 1 may be deduced from the first statement of Lemma 2. We preferred, however, to give the simple straightforward proof reproduced above.

[4] C. Löwner, Math. Z. **38**, 177 (1934).

[5] J. Bendat and S. Sherman, Trans. Am. Math. Soc. **79**, 58 (1955).

[6] M. Nakamura and H. Umegaki, Proc. Japan Acad. **37**, 149 (1961).

[7] C. Davis, Proc. Japan Acad. **37**, 533 (1961).

[8] I. E. Segal, J. Math. & Mech. **9**, 623 (1960).

The preceding lemmas may now be used to deduce the following results for the quantum entropy, specializations of which appear in Refs. 9 and 10.

Theorem 1: Let ρ be a statistical-mechanical state of the C^* algebra $\mathcal{A}$, and let $\{\rho_\Lambda\}$ be the corresponding system of density matrices. If $\mathcal{A}$ is the algebra for a fermion system, we assume further that ρ is an even state. Then the associated entropy $S(\rho_\Lambda)$ is a positive set function, i.e.,

$$S(\rho_\Lambda) \geq 0,$$

which is subadditive, i.e.,

$$S(\rho_{\Lambda_1 \cup \Lambda_2}) \leq S(\rho_{\Lambda_1}) + S(\rho_{\Lambda_2}),$$

if

$$\Lambda_1 \cap \Lambda_2 = \phi.$$

Further, if $\{\rho_\Lambda^{(1)}\}$ and $\{\rho_\Lambda^{(2)}\}$ are two families of density matrices and $1 \geq \alpha \geq 0$, then

$$\begin{aligned} \alpha S(\rho_\Lambda^{(1)}) + (1-\alpha) S(\rho_\Lambda^{(2)}) &\leq S[\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}] \\ &\leq \alpha S(\rho_\Lambda^{(1)}) + (1-\alpha)S(\rho_\Lambda^{(2)}) \\ &\quad - \alpha \log \alpha - (1-\alpha)\log(1-\alpha). \end{aligned}$$

Proof: The positivity of $S(\rho_\Lambda)$ is an immediate consequence of the normalization of ρ_Λ and the fact that

$$-\lambda \log \lambda \geq 0, \quad 1 \geq \lambda \geq 0.$$

The subadditivity property follows from Lemma 1, Proposition 1, and the identification $\mathcal{H} = \mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$, $A = \rho_{\Lambda_1 \cup \Lambda_2}$, and $B = \rho_{\Lambda_1} \otimes \rho_{\Lambda_2}$. The final inequality is a consequence of Lemma 2. The lower bound is immediately obtained from the first statement of that lemma, while the upper bound is obtained from the second statement as follows: We have

$$\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)} \geq \alpha\rho_\Lambda^{(1)} \geq 0,$$

and hence

$$\log[\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}] \geq \log \alpha\rho_\Lambda^{(1)}.$$

Thus

$$\begin{aligned} -\alpha \operatorname{Tr}[\rho_\Lambda^{(1)} \log(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)})] &\leq -\alpha \operatorname{Tr}[\rho_\Lambda^{(1)} \log \alpha\rho_\Lambda^{(1)}] \\ &= -\alpha \operatorname{Tr}[\rho_\Lambda^{(1)} \log \rho_\Lambda^{(1)}] - \alpha \log \alpha. \end{aligned}$$

Similarly,

$$\begin{aligned} &-(1-\alpha)\operatorname{Tr}[\rho_\Lambda^{(2)} \log(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)})] \\ &\leq -(1-\alpha)\operatorname{Tr}[\rho_\Lambda^{(2)} \log(1-\alpha)\rho_\Lambda^{(2)}] \\ &= -(1-\alpha)\operatorname{Tr}[\rho_\Lambda^{(2)} \log \rho_\Lambda^{(2)}] - (1-\alpha)\log(1-\alpha). \end{aligned}$$

Adding the last two inequalities yields the desired result.

4. MEAN ENTROPY—THE QUANTUM LATTICE SYSTEM

The next desirable aim would be to define an entropy per unit volume, or mean entropy, by establishing, under suitable restrictions, the existence of $S(\rho_\Lambda)/V(\Lambda)$ in the limit of Λ increasing such that the volume $V(\Lambda) \to \infty$. Unfortunately, we are at present able to do this only for a quantum lattice system, and even then it is not possible to establish the existence of the limit in the most desirable generality. A possible means of improving our results is discussed in the concluding section.

Let us define for $a = (a_1, \cdots, a_\nu) \in Z^\nu$ and $a_1 > 0, \cdots, a_\nu > 0$ the parallelepiped $\Lambda(a)$ by

$$\Lambda(a) = \{x \in Z^\nu; 0 < x_i \leq a_i \quad \text{for} \quad i = 1, 2, \cdots, \nu\}.$$

The measure (volume) $V[\Lambda(a)]$ of $\Lambda(a)$ is then given by $\prod_{i=1}^{\nu} a_i$.

Theorem 2: If the family $\rho = \{\rho_\Lambda\}$ of density matrices of a quantum lattice system satisfies the conditions of normalization, compatibility, and translation invariance, then the mean entropy

$$S(\rho) = \lim_{a_1, \ldots, a_\nu \to \infty} \frac{S(\rho_{\Lambda(a)})}{V(\Lambda(a))}$$

exists, and in fact

$$S(\rho) = \inf_{a_1, \ldots, a_\nu} \frac{S(\rho_{\Lambda(a)})}{V(\Lambda(a))}.$$

Further, $S(\rho)$ is an affine function. Explicitly, if $\rho^{(1)} = \{\rho_\Lambda^{(1)}\}$ and $\rho^{(2)} = \{\rho_\Lambda^{(2)}\}$ are two appropriate families of density matrices and $1 \geq \alpha \geq 0$, then

$$S[\alpha\rho^{(1)} + (1-\alpha)\rho^{(2)}] = \alpha S(\rho^{(1)}) + (1-\alpha)S(\rho^{(2)}).$$

Proof: By translation invariance, $S[\Lambda(a)]$ is a function of $a_1, \cdots, a_\nu$ only. Moreover, if we are dealing with a fermion system, translation invariance implies that the state ρ is even (see Sec. 2). But if we introduce a function $S(a_1, \cdots, a_\nu)$ through the definition

$$S(a_1, \cdots, a_\nu) = S[\Lambda(a)],$$

the subadditivity of $S(\Lambda)$ implies that $S(a_1, \cdots, a_\nu)$ is subadditive in each argument a_i $(1 \leq i \leq \nu)$ separately, i.e.,

$$\begin{aligned} S(a_1, \cdots, a_i^{(1)} + a_{i\nu}^{(2)}, \cdots, a_\nu) &= S(a_1, \cdots, a_i^{(1)}, \cdots a_\nu) \\ &\quad + S(a_i, \cdots, a_i^{(2)}, \cdots, a_\nu). \end{aligned}$$

[9] M. Delbrück and G. Molière, Abhandl. Preuss. Akad. P. 1 (1937).
[10] R. Jost, Helv. Phys. Acta **20**, 491 (1947).

A standard argument [cf. Ref. 11, Lemma A1] establishes the existence of

$$S(\rho) = \lim_{a_1, \cdots, a_\nu \to \infty} \frac{S(a_1, \cdots, a_\nu)}{a_1 a_2, \cdots, a_\nu} = \inf_{a_1, \cdots, a_\nu} \frac{S(a_1, \cdots, a_\nu)}{a_1 a_2, \cdots, a_\nu}.$$

The affine property of $S(\rho)$ follows from the last statement of Theorem 1, if one takes $\Lambda = \Lambda(a)$, divides by $V[\Lambda(a)]$, and takes the appropriate limit.

5. PROPERTIES OF THE MEAN ENTROPY

For fermion lattice systems and spin systems we can exploit the finite dimensionality of the $\mathcal{H}_\Lambda$'s to prove some additional properties of the mean entropy.

Theorem 3: Let $\mathcal{A}$ be the C^* algebra for a fermion lattice system or a spin lattice system. If x is a lattice point, let N denote the dimension of $\mathcal{H}_{\{x\}}$. Equip the set of states of $\mathcal{A}$ with the weak * topology. Then

(1) For any invariant state ρ of $\mathcal{A}$, $0 \leq S(\rho) \leq \operatorname{Log} N$.

(2) The mean entropy is an upper semicontinuous function on the set of invariant states of $\mathcal{A}$. If F is any closed subset of the set of invariant states of $\mathcal{A}$, then the restriction of the mean entropy to F attains its maximum.

(3) If ρ is an invariant state of $\mathcal{A}$, and if μ_ρ is the unique probability measure with barycenter ρ concentrated on the extremal invariant states of $\mathcal{A}$, then

$$S(\rho) = \int d\mu_\rho(\rho') S(\rho').$$

In physical language, statement 3 says that if ρ is an average of pure phases, then the mean entropy of ρ is the same average of the entropies of the pure phases making up ρ. For the existence and uniqueness of the measure μ_ρ, see Ref. 12, Theorem 2, or Ref. 13, Theorem 3. We remark that, under the hypotheses of this theorem, $\mathcal{A}$ is separable so there are no technical difficulties about the sense in which the measure is concentrated on the extremal invariant states.

Proof: For any finite set Λ of lattice points, the dimension of $\mathcal{H}_\Lambda$ is $N^{V(\Lambda)}$. Now

$$S(\rho_\Lambda) = -\sum_{i=1}^{N^{V(\Lambda)}} \lambda_i \log \lambda_i,$$

where the λ_i are the eigenvalues of ρ_Λ. By elementary estimates, if $\mu_1, \cdots, \mu_n$ are positive real numbers with $\sum_i \mu_i = 1$, then

$$-\sum_{i=1}^{n} \mu_i \log \mu_i \leq \log n.$$

Hence,

$$S(\rho_\Lambda) \leq \log (N^{V(\Lambda)}) = V(\Lambda) \log N.$$

Dividing by $V(\Lambda)$ and taking the limit of infinite volume gives

$$S(\rho) \leq \log N.$$

Since $S(\rho)$ is nonnegative by definition, we have proved part (1) of Theorem 3.

To prove part (2), observe first that the ρ_Λ's are continuous functions of ρ and that the eigenvalues of ρ_Λ vary continuously with ρ_Λ by perturbation theory. Since $-\lambda \log \lambda$ is a continuous function of λ,

$$S(\rho_\Lambda) = -\sum_i \lambda_i \log \lambda_i$$

is a continuous function of ρ. But

$$S(\rho) = \inf_\Lambda \left\{ \frac{S(\rho_\Lambda)}{V(\Lambda)} \right\},$$

where the infimum is to be taken over all rectangles. Thus, $S(\rho)$ is the infimum of a family of continuous functions and is therefore upper semicontinuous. In particular, if F is any closed set of invariant states on $\mathcal{A}$, then the restriction of S to F takes on its maximum, since any upper semicontinuous function on a compact set takes on its maximum.

Furthermore, since $S(\rho)$ is both affine and upper semicontinuous, it respects barycentric decompositions. More precisely, if μ is any probability measure on the set of invariant states of $\mathcal{A}$, and if the barycenter of μ is ρ, then

$$S(\rho) = \int d\mu(\rho') S(\rho').$$

(This follows from Lemma 10 of Ref. 14.) In particular, if μ_ρ is the unique decomposition of ρ into extremal invariant states,[15] then the above equation holds. This proves part (3) and completes the proof of the theorem.

6. CONCLUSION

While we have been able to obtain most of the desired results concerning the entropy of a quantum spin system, the position is less satisfactory in other cases. The main gap in the development is the failure to establish the existence of the mean entropy $S(\rho)$ under general circumstances. In classical statistical

[11] D. Ruelle, J. Math. Phys. **6**, 201 (1965).
[12] D. Kastler and D. W. Robinson, Commun. Math. Phys. **3**, 51 (1966).
[13] O. E. Lanford and D. Ruelle, J. Math. Phys. **8**, 1460 (1967).
[14] G. Choquet and P. A. Mayer, Ann. Inst. Fourier **13**, 139 (1963).
[15] Note that the uniqueness proofs given in Refs. 12 and 13 for such decompositions are valid even for Fermi systems. In the Fermi case, $\mathcal{A}$ is R^ν (or Z^ν) Abelian, in the sense of Ref. 13, as an argument similar to that appearing after Proposition 1 readily establishes.

mechanics[1] these existence problems were solved by showing that the entropy satisfied a condition of strong subadditivity. One could believe, and even support one's belief by heuristic physical arguments, that the same condition holds for the quantum entropy.

Conjecture: The quantum entropy $S(\rho_\Lambda)$ satisfies the inequality

$$S(\rho_{\Lambda_1\cup\Lambda_2}) + S(\rho_{\Lambda_1\cap\Lambda_2}) \leq S(\rho_{\Lambda_1}) + S(\rho_{\Lambda_2}).$$

A satisfactory discussion of the existence of the mean entropy would ensue, if this conjecture were proved. There would, however, still exist a problem in establishing a barycentric decomposition of the mean entropy in the general case because, although it would clearly be an affine function, it could not be expected to be upper semicontinuous.

We have not discussed in any detail the physical relevance of the mean entropy which we have introduced but postpone this to a forthcoming publication.[16]

ACKNOWLEDGMENTS

The authors are grateful to Professor D. Ruelle for many helpful and stimulating conversations. One of us (D. W. R.) would like to thank Professor R. Jost for a number of informative discussions. Finally, we would like to thank Professor P. Porcelli for his hospitality at the University of Louisiana during the Baton Rouge Symposium on C^* algebras where the present collaboration began.

[16] D. W. Robinson, Commun. Math. Phys. **6**, 151 (1967).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 9, NUMBER 7 JULY 1968

Parameter Differentiation of Exponential Operators and the Baker–Campbell–Hausdorff Formula

M. LUTZKY
U.S. Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

(Received 8 November 1967)

Parameter differentiation of exponential operators is used to derive a method for obtaining the Baker–Campbell–Hausdorff coefficients in a more explicit form than is available from the standard Hausdorff recursion formula. In passing, a derivation of the Hausdorff recursion formula is given which is simpler than the proof usually presented.

I. INTRODUCTION

The problem of solving the equation $e^z = e^x e^y$ for z, where x and y are noncommuting operators, frequently arises in physics. For instance, Weiss and Maradudin[1] discussed this problem in a study of x-ray scattering in crystals, and Snider[2] encountered it in the course of an investigation involving a linearization of the Boltzmann equation. The classical solution, given by Hausdorff,[3] involves an expansion of z into an infinite series of terms homogeneous in y, the successive terms being found from a recursion formula which utilizes the Hausdorff polarization operator. The recursion formula is known as the Baker–Campbell–Hausdorff formula (BCH), and has been discussed recently by several authors.[4] Unfortunately, the BCH formula is somewhat difficult to use for the computation of higher-order terms. In this paper, we use the method of parameter differentiation of exponential operators[5] to derive in a rather simple way a more explicit form for the BCH coefficients. In passing, we also show how the method may be used to provide a derivation of the BCH recursion formula that is somewhat simpler than the proof usually given.

II. PRELIMINARY DEFINITIONS AND FORMULAS

Our formulas will be considerably simplified by the use of the curly commutator bracket, recursively defined by

$$\{y, x^0\} = y, \tag{1}$$

$$\{y, x^{k+1}\} = [\{y, x^k\}, x]. \tag{2}$$

If $f(x)$ has a power-series expansion

$$f(x) = \sum_{k=0}^{\infty} a_k x^k,$$

[1] G. H. Weiss and A. A. Maradudin, J. Math. Phys. **3**, 771 (1962).
[2] R. F. Snider, J. Math. Phys. **5**, 1586 (1964).
[3] F. Hausdorff, Ber. Verhandl. Saechs. Akad. Wiss. Leipzig, Math.-Naturw. Kl. **58**, 19 (1906).
[4] W. Magnus, Commun. Pure Appl. Math. **7**, 649 (1954); J. Wei, J. Math. Phys. **4**, 1337 (1963); and Ref. 1.
[5] R. M. Wilcox, J. Math. Phys. **8**, 962 (1967).